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# Long-range coulomb interaction in ionic crystals

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## Abstract

Expressions have been proposed for calculating the matrix elements of the Coulomb interaction of p and d electrons in a chosen ion of a crystal with an infinite crystal lattice. The matrix elements have been calculated at Gaussian-type orbitals. The Coulomb interaction energy per molecular unit of the α'-NaV 2O 5 crystal has been calculated in the ionic approximation for homogeneous and chain orderings. It has been shown that the more correct determination of the energetic favorability of one or other ordering requires calculation of the Coulomb interaction energy with an infinite crystal lattice of electrons that are at different orbitals of the ion under consideration. © 2012 Pleiades Publishing, Ltd.

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